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A MODIFIED MULTI-CELL METHOD FOR SIMULATION OF ATMOSPHERIC TRANSPORT

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Abstract—A multi-cell method in which the cells are assumed to be open at the top (thus removing the need for the prescription of cell heights) is presented. The method is applied to the calculation of dispersion of SO_2 for a 2-h period in Nashville, Tennessee.

The multi-cell method for prediction of atmospheric dispersion of contaminants is simple to apply and usually yields results which compare favorably with those obtained by more cumbersome procedures. Recent applications of the method include the calculation of the concentration of particulate matter in Willamette Valley in Oregon (Reiquam, 1970a), sulfur in the atmosphere of northwest Europe (Reiquam, 1970b) and CO in the San Francisco Bay area (MacCracken *et al.*, 1971).

The basic assumption of the cell model is that the contaminants are readily carried and mixed by the wind and this results in a concentration field which, at any given time, is locally uniform. The region under study is divided into control cells for each of which, assuming the concentration to be uniform, the mass conservation equation can be solved to obtain local concentration. The assumption of uniform distribution obviously becomes better with decrease in the size of the cells. Because the wind direction is horizontal, uniform mixing in this direction is a plausible approximation. In the usual formulation of the cell model, however, the concentration distribution is taken to be uniform also in the vertical direction and a somewhat arbitrary height is assigned to the cells. This assumption is obviously unrealistic. In this note we describe a cell model in which a physically realistic vertical distribution is assumed. This does not affect the computational simplicity of the method. The modified method is used to calculate the dispersion of SO_2 in the atmosphere of Nashville, Tennessee, during a 2-h period, viz. 16:00–18:00 CST on 11 January 1959. This particular problem was chosen because more than usual amount of meteorological and emission inventory information is available for Nashville and because the same dispersion episode has previously been modelled by Randerson (1968, 1971), who integrated the three-dimensional diffusion equation numerically.

For simplicity, consider the emitting area to be divided into a grid of squares, each of which is regarded as a uniform area-source with a given strength. Each square of the grid is the base of a cell, (m,n), the indices m and n defining the position of the cell along the x- and y-axes respectively. The main assumption of the method is that the pollutants emitted from the surface are transported and mixed by the wind and this results in a concentration distribution which can be regarded as horizontally uniform over a short distance. Concentration within a cell after a given time interval can be evaluated by balancing the input into the cell, due to emission and advection, with the outflow into neighboring

cells. If $c(m,n)$ is the concentration of a particular non-reactive gas in the cell (m,n) and $Q(m,n)$ is its mass emitted per unit time into the cell, then the rate of change of $c(m,n)$ is given by the equation of conservation of mass in the cell (m,n):

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V(m,n)} c(m,n)\,\mathrm{d}V = -\int_{S(m,n)} c(m,n)\,\bar{U}(m,n)\cdot\mathrm{d}\bar{S} + Q(m,n) \tag{1}$$

where the volume and surface integrals are defined for the cell (m,n) and $\bar{U}(m,n)$ is the turbulent-mean wind velocity in the cell (m,n). The contribution of diffusive horizontal transport to equation (1) has been omitted because, although diffusion leads to the elimination of concentration gradient on a local scale, its effect on intercell transport is negligible in comparison with advection. If the base of a cell is a square of side h, then integration over the x- and y-coordinates in the equation gives:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^{l(m,n)} c(m,n)\,\mathrm{d}z = \frac{1}{h}\left[\int_0^{l(m-1,n)} c(m-1,n)\,u(m-1,n)\,\mathrm{d}z - \int_0^{l(m,n)} c(m,n)\,u(m,n)\,\mathrm{d}z\right]$$
$$+\frac{1}{h}\left[\int_0^{l(m,n-1)} c(m,n-1)\,v(m,n-1)\,\mathrm{d}z - \int_0^{l(m,n)} c(m,n)\,v(m,n)\,\mathrm{d}z\right] + \frac{Q(m,n)}{h^2} \tag{2}$$

where u and v are the x- and y-components of the mean wind velocity U and $l(m,n)$ is the height of the cell (m,n). We have taken u and v to be positive. The first term in the first square brackets represents the transfer of mass into the cell (m,n) from the next upwind cell $(m-1,n)$ in the x-direction, and the second term describes the loss of mass from the cell (m,n) due to the x-component of the wind. The terms in the second brackets similarly refer to transport in the y-direction.

To integrate over z we need to know the vertical distributions of the concentration c and the velocity $\bar{U}$. Possible vertical profiles of wind velocity have been studied in considerable detail and many theoretical and empirical formulations of them, which depend on the meteorological conditions, are available in the literature. In particular, it is known that under conditions of neutral stability the z-dependence of the wind velocity may be written in the form

$$U(z) = (U^*/k)\ln(z/z_0) \tag{3}$$

where U^*, k and z_0 are, respectively, the friction velocity, von Karman's constant and the roughness length. Wind observations in the Nashville episode under study are adequately reproduced by a profile of this form.

Related to the question of the vertical concentration distribution is that of fixing the height $l(m,n)$ of a cell. If a temperature inversion exists, which prevents the upward escape of the effluent material, then the height of the inversion appears to be a logical choice for l. If the inversion height is sufficiently low, such that the effluents are reflected from the inversion, the vertical concentration distribution may tend to be nearly uniform after a sufficiently long time has elapsed, as is assumed in usual formulations of the cell model. However, in the absence of an inversion the pollutants are free to diffuse upwards according to the prevailing atmospheric conditions and the vertical distribution would be far from uniform. In general, the vertical distribution would depend on many factors which are determined by the properties of the emission sources and those of the atmosphere and the terrain. Since the vertical distribution of pollutants emitted from a steady point source

is Gaussian, we may expect that it would not be grossly different in the case of a steady area source. We therefore assume that, in the absence of a temperature inversion,

$$c(z) = c_0 \exp(-z^2/2\sigma^2) \tag{4}$$

where c_0 is the concentration at ground level. Now, the vertical spread of the distribution is expected to increase as the pollutants from a particular source progress downwind. Hence for σ we adopt the empirical form:

$$\sigma(m,n) = a[x(m,n)]^b \tag{5}$$

where $x(m,n)$ is the distance of the cell (m,n) from the upwind edge of the emitting area and a and b are empirical constants. Values for a and b available in the literature are representative of atmospheric stability over open county. Because of larger surface roughness and heat island effects somewhat different values should be applicable to an urban atmosphere. For steady atmospheric conditions over a city we have adopted the values, following Gifford and Hanna (1971), usually quoted for "slightly stable" conditions. These are $a = 0.15$ and $b = 0.75$.

With the assumption of equation (4) a height need not be assigned and we can assume the cells to be open at the top, thus allowing unhindered vertical diffusion. In this limit, with $l \rightarrow \infty$, the mass conservation equation (2), becomes:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} c_0(m,n) = {} & c_0(m-1,n)\, I_u(m-1,n) - c_0(m,n)\, I_u(m,n) \\ & + c_0(m,n-1)\, I_v(m,n-1) - c_0(m,n)\, I_v(m,n) \\ & + \sqrt{\frac{2}{\pi}} \frac{Q(m,n)}{b^2 \sigma(m,n)}\end{aligned} \tag{6}$$

where

$$I_u(m,n) = \sqrt{\frac{2}{\pi}} \frac{1}{b\sigma(m,n)} \int_{L(m,n)}^{\infty} u(z) \exp[-z^2/2\sigma(m,n)^2]\, \mathrm{d}z$$

with a similar definition for I_v. The lower limit of the integral, $L(m,n)$, is the height assigned to the base of the cell (m,n) to take account of the topography of the terrain.

We now briefly describe the application of this modified cell model to the dispersion of SO_2 in the atmosphere of Nashville over a 2-h period. For a detailed description of the acquisition of data the reader is referred to Randerson (1968). Figure 1 shows the grid system and the area source strengths (g of SO_2 emitted s^{-1}) assigned to each cell. Each cell has a base of 1×1 mile. The wind field was determined from observations at 10-, 75- and 150-m levels and was found to fit closely the logarithmic distribution:

$$U = 0.48 \ln\left(\frac{Z - 15}{0.026}\right) \mathrm{m\,s^{-1}}; \quad Z > 16\ \mathrm{m}.$$

The average building height has been approximated to be 15 m. Observed wind speed and direction indicated no change in the field of air flow during the 2-h period. Consequently, wind speed and direction (from E.S.E. at 112.5°) were assumed to be steady. Topographically, Nashville is situated in a basin with hills to the south, west and north.

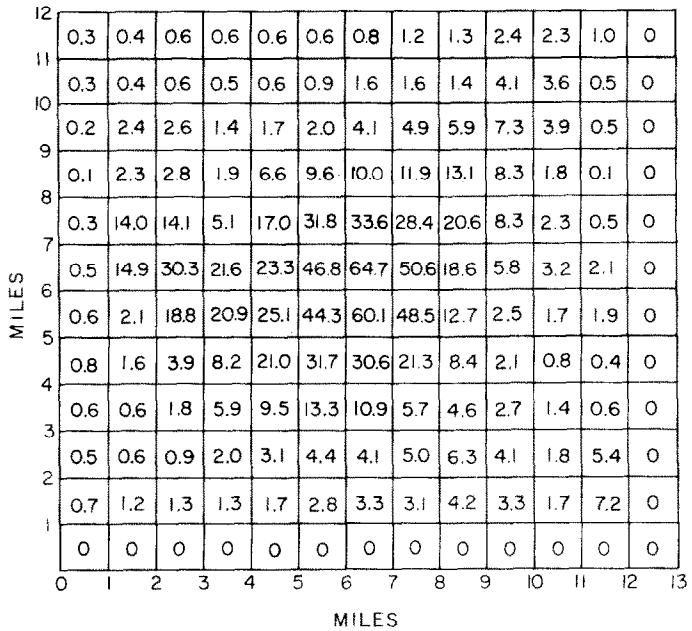

Fig. 1. The grid system for Nashville and the area source strength, in g of SO_2 mile^{-2} s^{-1} shown for each cell.

Initial values of SO_2 concentration at cell centers are estimates based on measurements at irregularly placed observation stations (Randerson, 1968). The evolution of SO_2 concentration in each cell is calculated for the 2-h period from equation (6) at successive small intervals of time. We assume that concentration at time $(t + \Delta t)$ is given by:

$$c(m, n; t + \Delta t) = \Delta t \frac{dc}{dt}(m, n; t) + c(m, n; t). \tag{7}$$

Terms of higher order in Δt may be easily included in the integration but the error due to their omission will be negligible as compared to the errors present in the calculation because of the inherently approximate nature of the data. The time interval Δt in our calculation was taken to be 5 s.

In the *conventional* cell model the concentration is assumed to be uniform vertically as well as horizontally. If the height of each cell is the same, viz. l, the mass conservation equation for the cell (m,n) becomes

$$\begin{aligned}\frac{d}{dt} c_0(m, n) = {} & \frac{1}{b}[c_0(m-1, n)\, u_{av}(m-1, n) - c_0(m, n)\, u_{av}(m, n)] \\ & + \frac{1}{b}[c_0(m, n-1)\, v_{av}(m, n-1) - c_0(m, n)\, v_{av}(m, n)] \\ & + \frac{Q(m, n)}{b^2 l}\end{aligned} \tag{8}$$

where $u_{av}(m,n)$ is the value of velocity component u averaged over the height of the cell (m,n), with a similar definition for $v_{av}(m,n)$. To test the dependence of the predicted con-

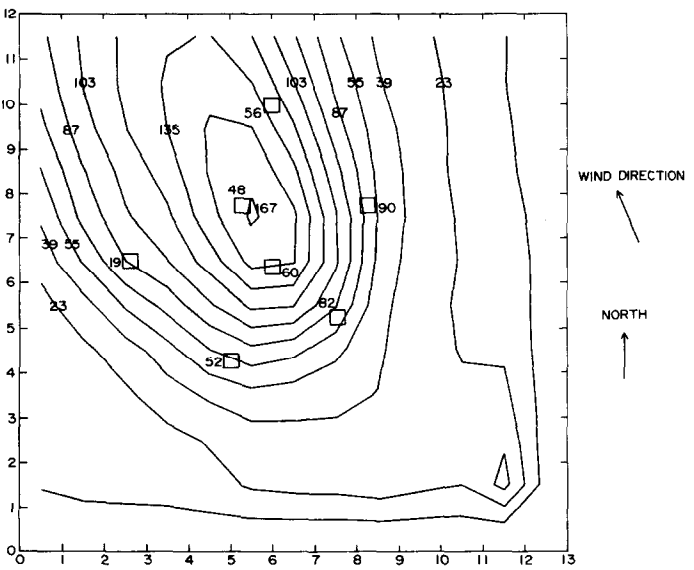

Fig. 2. Predicted contours of equal concentration of SO_2 in Nashville. Succeeding contours differ by 16 ppb. Numbered boxes indicate the locations of observation stations.

centration field on the height l, we did the calculation for Nashville for values of l equal to 100-, 125-, 150-, 175- and 200-m, according to equation (8). For a particular cell the predicted concentration at the end of the 2-h period decreases monotonically with increase in l. For instance, concentration decreases from 310 to 120 ppb at station (48), (see Fig. 2) and from 160 to 50 ppb at station (90), as l is increased from 100 to 200 m. The concentrations at different stations do not decrease at the same rate, so that the concentration distribution pattern looks notably different for different values of the cell height l. It is obvious therefore that the prescription of a cell height with a uniform vertical distribution introduces arbitrary errors in the calculation.

Surface concentrations of SO_2 at the end of the two hour period, as calculated by the *modified* cell method, namely equation (6), are shown in Fig. 2. The contours of equal concentration are obtained by linear interpolation between the values found for the cells.

The source distribution, Fig. 1, has a maximum near the center and a small maximum to the west of the center. These maxima result in local maxima of concentration in earlier parts of the 2-h period, but gradually they become less marked due to dispersion by the wind and the concentration pattern becomes aligned with the wind direction. The southern and eastern regions of Nashville have relatively clean air, the concentration of SO_2 being less than 40 ppb. The SO_2 spreads towards north and west where the concentration becomes higher; the maximum of concentration moves by only one cell in 2 h.

Sulfur dioxide concentration is observed at the seven stations shown in Fig. 2. The predicted concentrations are compared with the observed ones and those obtained by Randerson in Table 1. Concentrations are given as *mass fractions* in units of parts per billion (ppb)*. It may be noted that the observation stations are located at ground and therefore surface concentrations are listed. (The heights given for the stations by Randerson are

* Since the density of air is 1.23×10^3 g m^{-3} a pollutant concentration of 1.23×10^{-6} g m^{-3} is equivalent to 1 ppb.

Table 1. Comparison of observed and calculated concentrations at seven observing stations in Nashville. Concentrations are given in ppb (mass fractions)

Observation station number	Observed concentration	Present calculation	Numerical model of Randerson
19	128	87	110
48	299	160	140
52	64	70	88
56	152	130	20
60	460	150	310
82	290	80	92
90	90	63	59
Correlation coefficient		0·70	0·89
Mean relative error		−0·33	−0·53

elevations of the ground with respect to the base plane of the model.) It is seen that this model, like that of Randerson, generally underestimates the concentrations as compared to the observed values. The predictions of this model are within a factor of $\frac{1}{2}$ of the observed concentrations except for stations (60) and (82) where the discrepancy is larger. Randerson numerically solved the three-dimensional diffusion equation including the effects of diffusion, of vertical advection and of an exponential chemical decay. Although Randerson's method is potentially capable of very accurate results, his calculation is restricted to a height of 60 m only, even though some emission sources are located above 50 m. This ceiling at 60 m is probably responsible for the movement of the center of maximum concentration towards south–west in Randerson's calculation. The wind is from the south–east and the center is likely to move towards north–west, as observed in our calculation.

In conclusion, it may be said that the assumption of a uniform vertical distribution of concentration with an arbitrary cell height, which is a feature of the conventionally used multi-cell models, can be easily replaced by a more realistic assumption for the vertical distribution. This modification does not affect the computational simplicity of the multi-cell model and, our calculation for Nashville shows that, the modified method yields a concentration field which agrees well with the observed one in terms of qualitative features of distribution and the magnitude of relative error.

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